Version 0.2 - released Mar 26, 1993

As promised, full source is now available (in a separate file).

New Features:
Lots of little annoying bugs fixed. Most important, stick drawings now work correctly in the quick mode (there used to be a clipping problem).

An inspector panel with the following 3 sub-panels:
1. Atom Inspector - Allows viewing of atom coordinates and bonds. Selected atoms are labelled on the molecule. Bond lengths and angles and dihedral angles can now be measured.

2. Amino Acid Inspector - Molecules created or filtered through Alchemy are supported. All amino acids are located AND IDENTIFIED. The dihedrals of individual residues can be modified. The identified sequence can be transferred to the Protein Tool for display of a helical wheel diagram.

3. Atomic Table Inspector - Atom sizes and colors can now be modified

interactively. Changes are stored in the user's Library directory.

POV raytracer dump. You can now save your molecules as POV files as well as RIB files. POV is certainly much slower than RM, but it's more flexible. You can get POV from wuarchive.wustl.edu in /graphics/graphics/ray.

Buttons for setting the view size to several convenient values are provided (although the resize bar still works). If you are planning to generate pictures for display on other machines, this will help you get the size right. The "odd" sizes are for aspect ratio correction.

Known bugs and annoyances:
The radius used for drawing the atoms is the covalent radius from a Sargent-Welch periodic table Copr. 1980. I have checked several sources and can find no consistent values. If you disagree about a particular value, let me know ...

Large molecules in any of the renderman rendering modes can crash

the program. This behavior is quite unpredicable, sometimes the program continues to run without a display, sometimes it dies, and sometimes it kills the window server. This is acutally a bug in release 3.0 of the operating system, so I can't do anything about it.

Printing in "quick" mode doesn't work properly for the space filling model.

The ball and stick model is mostly unimplimented. It will only work with quick renderman. If you print or generate a RIB file, the "sticks" won't appear.

Currently the space filling, quick mode only supports the following atoms : H,C,N,O,P,S. Others will not appear.

I have no idea if color works correctly, since I only have a monochrome NeXT-Station to work with.

Currently document types aren't supported. You can't double click on a

molecule file and get it to open.

Only Alchemy molecules can be used with the dihedral angle routines (although you can always filter PDB files through alchemy).

The amino acid identifying routine has a few problems. Proline is incorrectly assigned as something else, and exotic amino acids (ones not in the internal table) may be mis-identified.

Future plans:
Currently the only bonds entered when PDB files are read are those specified in CONECT records. I plan to add a bond searching algorithm to fill in missing bonds.

More file formats???

Allow modification of bond angles, lengths and arbitrary dihedrals

I'd like to add some more protein analysis routines. Suggestions would be appreciated.

Better saving and printing options.

Support for more atoms in "Quick" mode.

(far future):
The ability to build molecules from scratch, ala alchemy.

Taking the entered protein sequence in the helical wheel diagram window and turning it into a molecule for display.

Version 0.1α - released Jan 31, 1993

Initial release - no source included.